Mean–field results on the Anderson impurity model out of equilibrium

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We investigate the mean–field phase diagram of the Anderson impurity model out of equilibrium. Generalising the unrestricted Hartree-Fock approach to the non-equilibrium situation we derive and analyse the system of equations defining the critical surface separating the magnetic regime from the non-magnetic one. An exact analytic solution for the phase boundary as a function of the applied voltage is found in the symmetric case. Surprisingly, we find that as soon as there is an asymmetry, even small, between the contacts, no finite voltage is able to destroy the magnetic regime which persists at arbitrary high voltages.

The field of 'Kondo physics' sprung from the crucial insight by Anderson into the formation of local magnetic moments in metals [1]. In Ref.[1], Anderson formulated a very simple model, now known as Anderson's impurity model (AIM), and showed that there is a critical value of Coulomb coupling (U_c) above which a local magnetic moment spontaneously forms (in the framework of a mean-field approximation). It was understood later (see [2], especially Chapter 5, and references therein), by using more sophisticated methods, that U_c is in fact a crossover rather than a sharp 'phase transition'. Nevertheless, the Anderson's original work [1] is a milestone for our understanding of the 'standard' Kondo problem. It still serves as a foundation for various more refined techniques, a notable example being the 'local moment approach' (LMA)[3].

In recent years, considerable theoretical interest in the non-equilibrium AIM developed, fuelled by experimental results on non-equilibrium transport in quantum dots where Kondo effect signatures were observed [4, 5]. The low bias voltage (V) limit of the AIM has been almost completely understood [6, 7] (perhaps the precise mechanism of 'dephasing' still being in need of some clarification [8]). When the voltage becomes larger than some characteristic scale (like the Kondo temperature), the situation is less clear. While there are some interesting results in the literature [9], no consistent theoretical method seems to be available to tackle the problem beyond the perturbation expansion in the on-site interaction, see e.g. Ref.[11]. In this paper we provide a starting point for one. Our objective is to generalise Anderson's original analysis [unrestricted Hartree–Fock (HF) approach] to the out of equilibrium model. Note that our starting point is complementary to that suggested in Ref.[10], which is appropriate for an expansion in the electron tunnelling amplitudes.

We start with the standard AIM Hamiltonian. It contains a single site with energy Δ described by electron creation and annihilation operators $d_\sigma^\dagger$, d_σ, where σ denotes the spin orientation. This site is coupled to two non-interacting electron systems $i = 1, 2$, which we shall also call 'leads'. Their dynamics is governed by the Hamiltonians $H_0[\psi_{i\sigma}]$, where $\psi_{i\sigma}$ are the corresponding electron field operators. The coupling of the leads to the impurity site takes place via hopping with energy-independent amplitudes $\gamma_{1,2}$,

$$
H = \sum_{\sigma=\uparrow,\downarrow} \left\{ \Delta d_\sigma^\dagger d_\sigma + \sum_{i=1,2} \left\{ H_0[\psi_{i\sigma}] + \right. \right.
$$
$$
\left. \left. + \gamma_i[d_\sigma^\dagger \psi_{i\sigma}(0) + \psi_{i\sigma}^\dagger(0)d_\sigma] \right\} \right\} + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow \,. \quad (1)
$$

The last term describes the on-site repulsion on the impurity. The cornerstone of the HF approach is the following approximation for this last term,

$$
U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow \rightarrow U(n_\uparrow d_\downarrow^\dagger d_\downarrow + n_\downarrow d_\uparrow^\dagger d_\uparrow) \,, \quad (2)
$$

where $n_\sigma = \langle d_\sigma^\dagger d_\sigma \rangle$ are the level population probabilities which have to be found self-consistently. The self-consistency equations are basically the population probabilities as functions of each other. In order to calculate them we first fix both n_σ. Then the full Hamiltonian separates with respect to spin degrees of freedom and can easily be diagonalised keeping in mind that n_σ are parameters. Since we are dealing with a non-equilibrium situation, the calculation of the population probabilities can only be accomplished using suitable modifications of the conventional equilibrium techniques. We decided to use the Keldysh formalism [12, 13]. Let us first define the local (taken at the site adjacent to the impurity) Green's function of the lead electrons (from now on we set the spacial coordinate to $x = 0$ and drop it hereafter),

$$
G_{i\sigma}(t - t') = -i\langle T_C \psi_{i\sigma}(t)\psi_{i\sigma}^\dagger(t') \rangle \,, \quad (3)
$$

where T_C denotes the time ordering operation along the closed Keldysh contour C consisting of the forward path C_-, running from $-\infty$ to ∞, and the backward path C_+ going the other way round. After an appropriate placement of the time variables, one can recover all usual Keldysh Green's functions from the generalised function (3), we use notation of Ref.[13]. We shall use only

the bare Green's functions of the lead electrons, i. e. those calculated without the tunnelling $\gamma_i = 0$ [the upper(lower) sign and subscript 1(2) corresponds to the left (right) lead],

$$
\begin{aligned}
G_{1(2)\sigma}^{--}(\omega) &= G_{1(2)\sigma}^{++}(\omega) = -i\frac{\rho_0}{2}\,\text{sgn}(\omega \pm V/2)\,, \\
G_{1(2)\sigma}^{-+}(\omega) &= i\,\rho_0\,\Theta(-\omega \mp V/2)\,, \\
G_{1(2)\sigma}^{+-}(\omega) &= -i\,\rho_0\,\Theta(\omega \pm V/2)\,,
\end{aligned}
\tag{4}
$$

where ρ_0 is the constant density of states in the leads and Θ denotes the Heaviside step function.

Green's functions of the impurity level are defined analogously and are denoted by D. The function $D_\sigma^{-+}(t-t')$ for $t - t' \to 0^-$, where 0^- is a negative infinitesimal, is related to the population of the level with spin projection σ,

$$
n_\sigma = \langle d_\sigma^\dagger(t) d_\sigma(t) \rangle = -i D_\sigma^{-+}(t-t')|_{t-t'=0^-}\,.
\tag{5}
$$

Therefore our goal is to calculate that particular Green's function. As already mentioned, the Hamiltonian in the HF approximation is quadratic, so that $D_\sigma^{-+}(t-t')$ can be calculated either using the re-summation technique of Ref.[14], or the non-equilibrium coherent state functional integrals [15, 16]. We choose the latter method because of its relative simplicity. The idea is to define a non-equilibrium counterpart of the partition function as a functional integral over all fields entering the Hamiltonian and integrate out all degrees of freedom apart of those corresponding to d_σ operators. The resulting expression will be quadratic in d_σ's which enables all correlation functions to be simply read off. Let us define the

following coherent state functional integral corresponding to a Keldysh partition function of the subsystem with spin orientation σ,

$$
\begin{aligned}
\mathcal{Z}_\sigma =\ & \int \mathcal{D}d_\sigma^* \mathcal{D}d_\sigma \prod_i \mathcal{D}\psi_{i\sigma}^* \mathcal{D}\psi_{i\sigma} \exp\Big\{ -i\sum_i S_i \\
& - i\int_C dt\, \Big[d_\sigma^*(t)(i\partial_t + \Delta + Un_{-\sigma})d_\sigma(t) \\
& + \sum_i \gamma_i[d_\sigma^*(t)\psi_{i\sigma}(t) + \psi_{i\sigma}^*(t)d_\sigma(t)] \Big] \Big\}\,,
\end{aligned}
\tag{6}
$$

where by abuse of terminology d_σ^*, d_σ and $\psi_{i\sigma}^*$, $\psi_{i\sigma}$ stand for the coherent state variables of the corresponding operators. S_i are the actions of the electrons in each lead. Notice that all time integrations are to be performed along the Keldysh contour C. Since the full action is Gaussian in the $\psi_{i\sigma}$ fields we can integrate them out thereby generating a non-local action for the impurity electrons. Separating time integrations along the $C_\pm$ branches we obtain the following expression,

$$
\begin{aligned}
\mathcal{Z}_\sigma = \int \mathcal{D}\vec{d}_\sigma^* \mathcal{D}\vec{d}_\sigma \exp\Big\{ &-i\int dt dt' \\
&\times \vec{d}_\sigma^*(t)\mathbf{D}_\sigma^{-1}(t-t')\vec{d}_\sigma(t') \Big\}\,,
\end{aligned}
\tag{7}
$$

with $\vec{d}_\sigma$ denoting a vector of $d_\sigma(t)$ for the time variable t on $C_\mp$. $\mathbf{D}_\sigma(t-t')$ is the quantity we are looking for – it is a matrix components of which give the Keldysh Green's functions of the impurity level operators. After the Fourier transformation its inverse is given by

$$
\mathbf{D}_\sigma^{-1}(\omega) = \begin{pmatrix} \omega + \Delta + Un_{-\sigma} + \sum_i \gamma_i^2 G_{i\sigma}^{--}(\omega) & \sum_i \gamma_i^2 G_{i\sigma}^{-+}(\omega) \\ \sum_i \gamma_i^2 G_{i\sigma}^{+-}(\omega) & -\omega - \Delta - Un_{-\sigma} + \sum_i \gamma_i^2 G_{i\sigma}^{++}(\omega) \end{pmatrix}
\tag{8}
$$

Therefore the Green's function that we are interested in is given by

$$
D_\sigma^{-+}(\omega) = -|\mathbf{D}_\sigma(\omega)|^{-1}\sum_i \gamma_i^2 G_{i\sigma}^{-+}(\omega)\,.
\tag{9}
$$

$|\mathbf{D}_\sigma(\omega)|$ denotes the determinant of the matrix (8). Inserting Eqs.(4) into (9) yields

$$
D_\sigma^{-+}(\omega) = i\frac{\Gamma_1\Theta(-\omega+V/2) + \Gamma_2\Theta(-\omega-V/2)}{(\omega + \Delta + Un_{-\sigma})^2 + (\Gamma_1 + \Gamma_2)^2}\,,
\tag{10}
$$

where $\Gamma_i = \pi\rho_0\gamma_i^2$. Finally, according to Eq. (5), n_σ is just the energy integral of (10) with an appropriate prefactor,

$$
n_\sigma = \frac{\delta}{\pi}\cot^{-1}\left(\frac{\Delta - V/2 + Un_{-\sigma}}{\Gamma}\right)
$$

$$
+ \frac{1-\delta}{\pi}\cot^{-1}\left(\frac{\Delta + V/2 + Un_{-\sigma}}{\Gamma}\right)\,,
\tag{11}
$$

where $\Gamma = \Gamma_1 + \Gamma_2$ and $\delta = \Gamma_1/\Gamma$ is the asymmetry parameter. Eqs.(11) are the self-consistency equations for the impurity level population probabilities. In the equilibrium case these equations reduce to Eqs.(27) of Ref.[1]. Introducing dimensionless parameters $x = -\Delta/U$, $y = U/\Gamma$ and $z = V/2\Gamma$ the above equations simplify to

$$
\begin{aligned}
n_\sigma =\ & \frac{\delta}{\pi}\cot^{-1}[y(n_{-\sigma} - x) - z] \\
& + \frac{1-\delta}{\pi}\cot^{-1}[y(n_{-\sigma} - x) + z]\,.
\end{aligned}
\tag{12}
$$

It is reasonable to expect that both the magnetic ($n_\sigma \neq n_{-\sigma}$) and the non-magnetic ($n_\sigma = n_{-\sigma}$) regimes still exist

for small z. The critical (x–y) curve, however, acquires an additional dimension (z) and thus becomes a critical surface. Our goal is to determine its shape. Proceeding along the lines of Ref.[1], we derive the equations for the surface. The first equation is essentially given by Eq.(12) for $n_\sigma = n_{-\sigma} = n_c$ and the second one is just its derivative with respect to n_c,

$$\begin{cases} \pi n_c = \delta \cot^{-1}[y_c(n_c - x_c) - z] + (1-\delta)\cot^{-1}[y_c(n_c - x_c) + z], \\ \pi/y_c = \delta\{1 + [y_c(n_c - x_c) - z]^2\}^{-1} + (1-\delta)\{1 + [y_c(n_c - x_c) + z]^2\}^{-1}, \end{cases}$$ (13)

where the subscript 'c' stands for the parameter of the critical surface. Obviously, in the equilibrium situation ($z = 0$) the asymmetry does not matter and one obtains the result of Ref. [1],

$$\begin{cases} x_c = n_c - \sin(2\pi n_c)/2\pi, \\ \pi/y_c = \sin^2(\pi n_c), \end{cases}$$ (14)

where n_c plays the role of a parametrisation and runs from 0 to 1, see Fig.1. Out of equilibrium, the equations (13) cannot be reduced in the same way and need to be solved numerically in the general case. Yet it is possible to investigate some interesting special cases analytically.

Let us first concentrate on the symmetric case $\delta = 1/2$. Then Eqs.(13) are obviously symmetric with respect to transformation $z \to -z$, so that we can restrict ourselves to positive z. Next we observe that, just as in equilibrium, there is an additional symmetry with respect to the axis $x = 1/2$: $x_c \leftrightarrow 1 - x_c$ (which, of course, corresponds to $n_c \leftrightarrow 1 - n_c$). Moreover, at the special point $x_c = 1/2$ Eqs.(13) can be solved exactly. The first of them fixes n_c to $1/2$ but does not impose any restrictions on z, so that from the second equation we obtain,

$$y_c = \pi(1 + z^2).$$ (15)

The main feature of this result is that, at least on the line $x_c = 1/2$, the magnetic phase is never completely destroyed by the applied voltage. Another remarkable property of the phase diagram which can be extracted from the result (15) is the fact that although the point $x_c = 1/2$ on the equilibrium curve corresponds to the lowest critical interaction strength U and therefore to the most favorable condition for the magnetic phase to emerge, it does not possess that property above the critical value $z^* = 1/\sqrt{3}$. This can be seen from the lowest order expansion of Eq. (15) in powers of $x_c - 1/2$,

$$y_c \approx \pi(1 + z^2)\left[1 + \frac{\pi^2}{4}(1 - 3z^2)(x_c - 1/2)^2\right],$$ (16)

which means that the phase diagram develops a dip toward the x axis at $z > z^*$, see Fig.1.

Let us now analyse the behaviour of the critical curves for small x_c. In that limit n_c happens to be small as well so that we can regard it as a good expansion parameter.
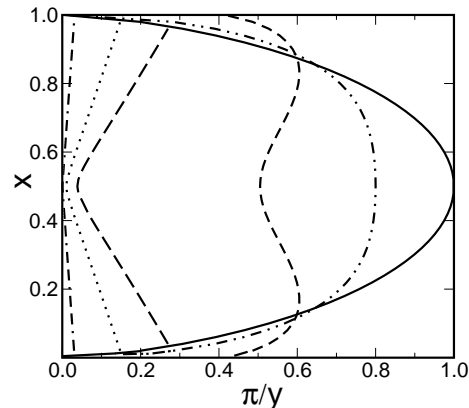

FIG. 1: Mean–field phase diagram of the AIM in the symmetric case $\delta = 1/2$ evaluated numerically using Eqs.(13) for different voltage parameters z. From right to left along the $x_c = 1/2$ line: $z = 0, 0.5, 1, 5, 10, 50$. The magnetic phase is bounded by the curves and the axis of ordinates.

From the first of Eqs.(13) one can easily see that in such a situation the $\cot^{-1}$ functions are vanishing so that it can be solved after an asymptotic expansion of trigonometric functions. The result is $y_c(n_c - x_c) = (\pi n_c)^{-1} + \pi n_c z^2$. It can be plugged into the second equation and the whole procedure results in the following parametric representation,

$$\begin{cases} x_c = n_c - \left[(\pi^2 n_c)^{-1} + n_c z^2\right](\pi/y_c), \\ \pi/y_c = \sum_{p=\pm}\{1 + [(\pi n_c)^{-1} + \pi n_c z^2 + pz]^2\}^{-1}. \end{cases}$$ (17)

Being plotted numerically this curve starts from the origin and never crosses the $x_c = 0$ axis again unless $z > 0.707 \approx 1/\sqrt{2}$. Therefore in this latter situation the finite voltage encourages the system to become magnetic. This fact also reveals itself as a 'squeezing' of the magnetic region toward the lines $x_c = 0, 1$, see Fig.1.

To summarise the effects of the voltage in the symmetric case ($\delta = 1$), the equilibrium conditions for the stability of the magnetic phase remain qualitatively intact as long as $z < z^*$. For larger voltages, $z > z^*$,
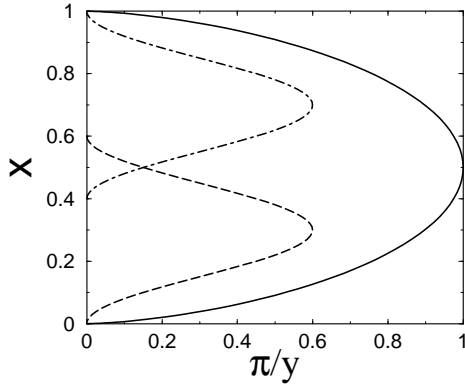
FIG. 2: Mean–field phase diagram of the AIM in the asymmetric case $\delta = 0.4$ evaluated numerically using Eqs.(19). Dashed line corresponds to high negative voltages and dot-dashed one represents the limit of high positive voltages. For comparison: the solid line is the equilibrium $z = 0$ critical curve.

it becomes favourable to measure the dot level Δ from either of the two shifted chemical potentials $\mu_{R,L}$ in order to preserve the local moment. Hence the dip in the phase diagram. Yet, when V is sent to infinity, the magnetic phase completely disappears in the symmetric case. Surpisingly, the magnetic phase persists up to $V = \infty$ in the asymmetric case ($\delta \neq 1$), which we investigate next.

The limit of large applied voltage can also be investigated analytically. However, from the physical point of view it is more convenient to interpret the results for a system where the voltage is applied asymmetrically. Such situation takes place e.g. if we shift our voltage variable to zero in one channel and to $2z$ in the other one. Sending the voltage to infinity simplifies the first equation of the system (13) to

$$y_c(n_c - x_c) = \cot\left(\pi\frac{n_c - \delta}{1 - \delta}\right), \qquad (18)$$

from which we immediately see that $\delta < n_c < 1$. Insertion of Eq. (18) into the second one of the system (13) yields the following parametric representation,

$$
\begin{cases}
x_c = n_c - (1 - \delta)\sin[2\pi(n_c - \delta)/(1 - \delta)]/2\pi\,, \\
\pi/y_c = (1 - \delta)\sin^2[\pi(n_c - \delta)/(1 - \delta)]\,.
\end{cases}
\qquad (19)
$$

At large negative voltages the picture is changed only by the transformation $x_c \to 1 - x_c$. Sending the applied voltage to infinity effectively corresponds to a removal the weaker lead. As one would expect in his case the critical curve has then exactly the same shape as the curve in equilibrium apart of a renormalisation by the asymmetry parameter δ and a shift of the dot population n_c, see Fig.2.

To conclude, we investigated the mean–field phase diagram of the non-equilibrium Anderson impurity model by means of the unrestricted Hartree-Fock approximation. We present an analytic expression for the critical curve between the magnetic and non-magnetic phases in the symmetric case when the level energy $-\Delta$ is equal to the half of the on-site interaction constant U. It turns out that above some critical value of the applied voltage $V > 2\Gamma/\sqrt{3}$ the critical curve acquires a dip which means that the most favorable conditions for the magnetic phase to form change. We show that the magnetic phase exists at *arbitrary* voltages in the *asymmetric* case. We consider our HF solution as an appropriate starting point for further investigations into the problem including fluctuations in the functional integral approach or through a suitable generalisation of the LMA.

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